The solution of Schrodinger equation in bispherical coordinate with Kratzer potential using Hypergeometry method

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Abstract: The Hypergeometry method can be used to solve the Schrodinger equation in bisperical coordinate for Kratzer potential. By substituting Laplacian in bisperical coordinate, the new wave function, and potential parameters, the Schrodinger equation was reduced to the second order of Hypergeometry function equation which is used to determine the energy and un-normalized wave function equation. Energy spectrum was calculated using Matlab software and the un-normalized wave function was expressed in hypergeometry form.

Keywords: Schrodinger equation, bispherical coordinate, Kratzer potential, Hypergeometry method

1. Introduction

An analytical solution of the radial Schrodinger equation is of high importance in quantum mechanics because the wave functions and energy contain all the important information needed to describe quantum systems (Bayrak et al., 2006). The solution of Scrodinger equation for some potential have been investigated by some authors using the factorization method (Sadeghi, 2007), supersymmetry of quantum mechanics (SUSYQM) (Ahmadov et al., 2017; Ahmadov et al., 2018), Asymptotic Iteration Method (AIM) (Bayrak et al., 2006; Falaye, 2012; Bayrak & Boztosun, 2007), Nikiforov–Uvarov method (NU) (Edet et al., 2019; Berkdemir & Han, 2005; Ikot et al., 2013; Okon et al., 2017), and Hypergeometry (Hidayat et al., 2019). One method used in this study is the Hypergeometry method. The Hypergeometry method can be applied to several potentials, specifically for potential invariant forms, such as Kratzer, Gendenhstein, Morse, Pöschl-Teller, Morse Rosen, Scarf, Manning Rosen, Eckart, Wood-Saxon and Top Symmetrical potential (Suparmi, 2011).

In this study, the potential is used the Kratzer potential. Kratzer potential is mostly applied in atomic physics, molecular physics, and quantum chemistry (Sadeghi, 2007). Kratzer potential is used to describing the interaction of molecular structures in quantum mechanics. Kratzer's potential consists of a long-range attraction and a repulsive part. The integration of the Kratzer potential can be used to determine the eigenvalues of vibrational and rotational energy. The Kratzer potential is known as the infinity approach when the

internuclear distance approaches are zero because the repulsion is between potential molecules. the distance of the internuclear molecule approaches infinity because the potential decomposes to zero (Bayrak et al., 2006).

This paper covers several sections, the solution of Schrodinger equation in bispherical coordinate and Hypergeometry method in section 2, The result and discussion about the result energy spectrum and the unnormalized wave function were expressed in Hypergeometry terms in section 3, and conclusion in section 4.

2. Research Methods

2.1. The solution of the Schrodinger equation in bispherical coordinate

The general of time-independent Schrodinger equation with mass (m) and vector potential $V(\mu)$ is given by (Taskin & Kocak, 2010)

$$\left[-\frac{\mathbf{h}^2}{2m}\nabla^2 + V(\mu)\right]\psi = E\psi \tag{1}$$

From the formulas for the gradient and divergence, we can form the Laplacian the Laplacian in curvilinear coordinate is given as (Arfken et al., 2005)

$$\nabla^2 \psi = \nabla \cdot \nabla \psi = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial q_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial \psi}{\partial q_1} \right) + \frac{\partial}{\partial q_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial \psi}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial \psi}{\partial q_3} \right) \right]$$
(2)

The scale factor of the bisperical coordinates is defined as follows (Gongora & Rev, 1996; Gilbert & Giacomin, 2019)

$$h_{\eta} = h_{\mu} = \frac{a}{\cosh \mu - \cos \eta} \tag{3a}$$

$$h_{\phi} = \frac{a \sin \eta}{\cosh \mu - \cos \eta} \tag{3b}$$

Equation (3a) and (3b) were inserted into equation (2), so we get operator Laplacian in bispherical coordinate is given as

$$\nabla^2 \psi = \frac{1}{h_{\mu}^3} \left[\frac{\partial}{\partial \mu} \left(h_{\mu} \frac{\partial \psi}{\partial \mu} \right) + \frac{1}{\sin \eta} \frac{\partial}{\partial \eta} \left(h_{\mu} \sin \eta \frac{\partial \psi}{\partial \eta} \right) + \frac{h_{\mu}}{\sin^2 \eta} \frac{\partial^2 \psi}{\partial \phi^2} \right]$$
(4)

Equation (4) will be simplified by introducing new wave function as $\psi = \sqrt{\cosh \mu - \cos \eta} F$ that it was reduced to

$$\nabla^2 \psi = \frac{\left(\cosh \mu - \cos \eta\right)^{5/2}}{a^2} \left[\frac{\partial^2 F}{\partial \mu^2} + \frac{1}{\sin \eta} \frac{\partial}{\partial \eta} \left(\sin \eta \frac{\partial F}{\partial \eta}\right) + \frac{1}{\sin^2 \eta} \frac{\partial^2 F}{\partial \phi^2} - \frac{F}{4} \right]$$
(5)

Equation (5) and $\psi = \sqrt{\cosh \mu - \cos \eta F}$ were inserted into equation (1) is given as

$$\frac{\left(\cosh\mu - \cos\eta\right)^{2}}{a^{2}} \left[-\frac{F}{4} + \frac{\partial^{2}F}{\partial\mu^{2}} + \frac{1}{\sin\eta} \frac{\partial}{\partial\eta} \left(\sin\eta \frac{\partial F}{\partial\eta}\right) + \frac{1}{\sin^{2}\eta} \frac{\partial^{2}F}{\partial\phi^{2}} \right] - \frac{2m}{h^{2}} V(\mu) F = -\frac{2m}{h^{2}} EF$$
(6)

Equation (6) is a Schrodinger equation in bispherical coordinate that can be solved analytically and exactly by introducing variable mass

$$m = \frac{m_0 \left(\cosh \mu - \cos \eta\right)^2}{a^2} \tag{7}$$

Where m_0 is reduced mass parameter. Equation (7) was inserted into equation (6), we get

$$\frac{\partial^2 F}{\partial \mu^2} + \frac{1}{\sin \eta} \frac{\partial}{\partial \eta} \left(\sin \eta \frac{\partial F}{\partial \eta} \right) + \frac{1}{\sin^2 \eta} \frac{\partial^2 F}{\partial \phi^2} - \frac{2m_0}{h^2} V(\mu) F - \left(\frac{1}{4} - \frac{2m_0}{h^2} E \right) F = 0$$
(8)

Equation (7) can be solved using the variable separation method and setting the new wave function $F = M(\mu)H(\eta)P(\phi)$ to obtain three parts with different direction as μ , η , ϕ in Schrödinger equation in bispherical coordinates is gives as

$$\frac{\partial^2 M}{\partial \mu^2} - \frac{2m_0}{h^2} V(\mu) M - \left(\frac{1}{4} - \frac{2m_0}{h^2}E\right) M = -\frac{1}{H\sin\eta} \frac{\partial}{\partial\eta} \left(\sin\eta \frac{\partial H}{\partial\eta}\right) - \frac{1}{P\sin^2\eta} \frac{\partial^2 P}{\partial\phi^2} = \lambda_1$$
(9)
$$-\frac{\sin\eta}{H} \frac{\partial}{\partial\eta} \left(\sin\eta \frac{\partial H}{\partial\eta}\right) + \frac{2m_0}{h^2} V(\eta) \sin^2\eta - \lambda_1 \sin^2\eta = \lambda_2$$
(10)

$$\frac{\partial^2 P}{\partial \phi^2} - \frac{2m_0}{h^2} V(\phi) P = \lambda_2 P \tag{11}$$

The radial part of Schrodinger equation in bispherical coordinate in Equation (9) was simplified to

$$\frac{\partial^2 M}{\partial \mu^2} - \frac{2m_0}{h^2} V(\mu) M - E' M = 0$$
(12)

with

$$E' = \left(\frac{1+4\lambda_1}{4} - \frac{2m_0}{h^2}E\right)$$
(13)

2.2. Hypergeometry methods

The principles of Hypergeometry method is substituted with new variable and parameter to obtain a second-order differential equation of Hypergeometry function which is expressed by (Suparmi, 2011; Suparmi et al., 2019).

$$z(1-z)\frac{d^{2}\phi}{dz^{2}} + (c - (a+b+1)z)\frac{d\phi}{dz} - ab\phi = 0$$
(14)

Equation (14) has two regular singulars points at z = 0 and z = 1, and an irregular singular point in $z = \infty$. By choosing a simple form, the solution of equation (14) is expressed in a series form around point z = 0 is given as (Suparmi, 2011; Suparmi et al., 2019)

$$\phi = z^s \sum a_n z^n \tag{15}$$

The solution form of the Hypergeometry differential equation in Equation (14) is given as (Suparmi, 2011).

$$\phi_{1}(z) = {}_{2}F_{1}(a,b,c;z) = \sum_{n=0}^{\infty} \frac{(a)_{n}(b)_{n}}{(c)_{n}n!} z^{n}$$
(16)

With,

$$(a)_{n} = a(a+1)(a+2)(a+3)....(a+n-1) \operatorname{dan} (a)_{o} = 1$$
(17)

The energy spectrum level is obtained when the solution of Equation (16) has form of polynomial rank a = -n or b = -n.

3. Result and Disscussion

Kratzer potential is defined by [7,17-18]

$$V(\mu) = -\frac{V_1}{\mu} + \frac{V_2}{\mu^2}$$
(18)

With $V_1 = 2D_e a$ and $V_2 = D_e a^2$. Where D_e is the dissociation energy and a is the equilibrium internuclear separation.

We employ the approximation scheme to get rid of the centrifugal barrier as (Edet et al., 2019; Greene & Aldrich, 1976).

$$\frac{1}{\mu^2} \approx \frac{q^2}{\left(1 - e^{-q\mu}\right)^2} \text{ and } \frac{1}{\mu} \approx \frac{q}{\left(1 - e^{-q\mu}\right)}$$
(19)

Equation (19) was inserted into Equation (18) was given as

$$V(\mu) = -\frac{V_1 q}{\left(1 - e^{-q\mu}\right)} + \frac{V_2 q^2}{\left(1 - e^{-q\mu}\right)^2}$$
(20)

Equation (20) can be changed using the hyperbolic function rule was given as (Spigel, 1968)

$$-\frac{V_1q}{\left(1-e^{-q\mu}\right)} = -\frac{V_1q}{2} \operatorname{coth}\left(\frac{q\mu}{2}\right) - \frac{V_1q}{2}$$
(21)

$$\frac{V_2 q^2}{\left(1 - e^{-q\mu}\right)^2} = \frac{V_2 q^2}{4} \cos ech^2 \left(\frac{q\mu}{2}\right) + \frac{V_2 q^2}{2} \coth\left(\frac{q\mu}{2}\right) + \frac{V_2 q^2}{2}$$
(22)

Equation (21) and (22) were inserted into equation (12), we obtain

$$\frac{\partial^2 M}{\partial \mu^2} - \frac{m_0 q^2 V_2}{2h^2} \cos ech^2 \left(\frac{q\mu}{2}\right) + \left[\frac{\frac{m_0 q V_1}{h^2}}{-\frac{m_0 q^2 V_2}{h^2}}\right] \coth\left(\frac{q\mu}{2}\right) M - \left(-\frac{\frac{m_0 q V_1}{h^2}}{-\frac{m_0 q^2 V_2}{h^2}}\right) M = 0$$
(23)

Equation (23) can be solved by Hypergeometry method with variable and parameter substitution like using Manning Rosen potential. In equation (23) with approximation variable like in Manning Rosen, we have relationship equation (Suparmi, 2011):

$$v(v-1) = \frac{m_0 q^2 V_2}{2h^2}$$
(24a)

$$2\delta = \frac{m_0 q V_1}{h^2} - \frac{m_0 q^2 V_2}{h^2}$$
(24b)

$$k^{2} = -\frac{m_{0}qV_{1}}{h^{2}} + \frac{m_{0}q^{2}V_{2}}{h^{2}} + E'$$
(24c)

Equation (24a)-(24c) were inserted into equation (23), we get

$$\frac{\partial^2 M}{\partial \mu^2} - v(v-1)\cos ech^2\left(\frac{q\mu}{2}\right) + 2\delta \coth\left(\frac{q\mu}{2}\right)M - k^2M = 0$$
(25)

Equation (25) can be solved by using variable and parameter approximation was given as

$$\operatorname{coth}\left(\frac{q\mu}{2}\right) = 1 - 2z \text{ and } \cos ech^2\left(\frac{q\mu}{2}\right) = 4z(z-1)$$
(26)

$$\frac{d}{d\mu} = \frac{d}{dz}\frac{dz}{d\mu} = qz(z-1)\frac{d}{dz}; \ \frac{d^2}{d\mu^2} = q^2 z^2 (z-1)^2 \frac{d^2}{dz^2} + q^2 z(z-1)(2z-1)\frac{d}{dz}$$
(27)

Equation (26)-(27) were applied in equation (25), we get

$$q^{2} z^{2} (z-1)^{2} \frac{d^{2} M}{dz^{2}} + q^{2} z(z-1)(2z-1) \frac{dM}{dz} - 4v(v-1) z(z-1) M$$

$$+ 2\delta(1-2z) M - k^{2} M = 0$$
(28)

The left and right segments in Equation (28) was divided $q^2 z(z-1)$, we get

$$z(z-1)\frac{d^2M}{dz^2} + (2z-1)\frac{dM}{dz} - \left[\frac{4v(v-1)}{q^2} - \frac{2\delta(1-2z)}{q^2z(z-1)} + \frac{k^2}{q^2z(z-1)}\right]M = 0$$
(29)

By setting z-1 = -(1-z) and 2z-1 = -(1-2z) in Equation (29) was given as

$$-z(1-z)\frac{d^{2}M}{dz^{2}} - (1-2z)\frac{dM}{dz} - \left[\frac{4v(v-1)}{q^{2}} + \frac{2\delta(1-2z)}{q^{2}z(1-z)} - \frac{k^{2}}{q^{2}z(1-z)}\right]M = 0$$
(30)

The left and right segments in Equation (30) was multiplied (-1) was given as

$$z(1-z)\frac{d^2M}{dz^2} + (1-2z)\frac{dM}{dz} + \left[\frac{4v(v-1)}{q^2} + \frac{2\delta(1-2z)}{q^2z(1-z)} - \frac{k^2}{q^2z(1-z)}\right]M = 0$$
(31)

By setting the new parameters in Equation (31), we have

$$v'(v'-1) = \frac{4v(v-1)}{q^2}$$
(32a)

$$\frac{\delta}{q^2} = \delta' \tag{32b}$$

$$k'^{2} = \frac{k^{2}}{q^{2}}$$
(32c)

Equation (32a)-(32c) were inserted into equation (31), we obtain

$$z(1-z)\frac{d^2M}{dz^2} + (1-2z)\frac{dM}{dz} + v'(v'-1) + \frac{2\delta'(1-2z)}{z(1-z)} - \frac{k'^2}{z(1-z)} = 0$$
(33)

Equation (33) was simplified to

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$$-z)\frac{d^{2}M}{dz^{2}} + (1-2z)\frac{dM}{dz} + \left[v'(v'-1) - \frac{-2\delta' + k'^{2}}{z} - \frac{2\delta' + k'^{2}}{(1-z)}\right]M = 0$$
(34)

By setting the new wave function and new parameter were given as

$$M = z^{\alpha} \left(1 - z\right)^{\beta} f(z), \qquad (35a)$$

$$-2\delta' + k'^2 = \alpha^2 \text{ and } 2\delta' + k'^2 = \beta^2$$
 (35b)

Equation (35a) and (35b) were inserted into Equation (34), we get the second-order Hypergeometry function like equation (14) is given as

$$z(1-z)f''(z) + [(2\alpha+1) - (2\alpha+2\beta+2)z]f'(z) + [v'(v'-1) - (\alpha+\beta)(\alpha+\beta+1)]f(z) = 0$$
(36)

By setting new parameter in Equation (36) like Equation (14), we have

$$a' = \alpha + \beta - v' + 1; \ b' = \alpha + \beta + v'; \text{ and } c' = 2\alpha + 1$$
 (37)

Equation (37) was choosen a' = -n, we get

$$a' = \alpha + \beta - v' + 1 = -n \rightarrow (\alpha + \beta)^2 = (v' - 1 - n)^2$$
 (38)

Equation (35b) was inserted into Equation (38), we obtain

$$2k'^{2} + 2\sqrt{\left(k'^{4} - 4\delta'^{2}\right)} = \left(v' - 1 - n\right)^{2}$$
(39)

Equation (39) was simplified to

$$k'^{2} = \frac{\left(v'-1-n\right)^{2}}{4} + \frac{4\delta'^{2}}{\left(v'-1-n\right)^{2}}$$
(40)

Equation (13), (24c), and (32c) were applied in Equation (40), we obtain

$$E = \frac{\left(-V_1 q + V_2 q^2\right)}{2} + \frac{h^2}{8m_0} + \frac{h^2 \lambda_1}{2m_0} - \frac{h^2 q^2}{2m_0} \frac{\left(v' - 1 - n\right)^2}{4} - \frac{h^2 q^2}{2m_0} \frac{4\delta'^2}{\left(v' - 1 - n\right)^2}$$
(41)

With,

$$v'(v'-1) = \frac{4v(v-1)}{q^2} = \frac{4\left(\frac{m_0q^2V_2}{2h^2}\right)}{q^2} = \frac{2m_0V_2}{h^2} \to v' = \sqrt{\frac{2m_0q^2V_2}{h^2} + \frac{1}{4}} + \frac{1}{2}$$
(42)

$$\frac{\delta}{q^2} = \delta' \to \delta' = \frac{\frac{m_0}{2h^2} \left(qV_1 - q^2 V_2 \right)}{q^2} = \frac{m_0}{2q^2 h^2} \left(qV_1 - q^2 V_2 \right)$$
(43)

Equation (41) is the energy spectrum equation of the Kratzer potential in bispherical coordinates using the Hypergeometry method.

Furthermore, the wave function equation for the Schrodinger equation in bispherical coordinate with Hypergeometry method for Kratzer potential has a solution with application Equation (16) in Equation (35a), we get (Suparmi, 2011; Spigel, 1968).

$$M = z^{\alpha} (1-z)^{\beta} f(z) = z^{\alpha} (1-z)^{\beta} {}_{2} F_{1}(a',b',c',z)$$
(44)

Equation (35b) was inserted into Equation (40), so we get new parameters α dan β as follows

$$\alpha = \frac{1}{2} \left(v' - 1 - n - \frac{4\delta'}{v' - 1 - n} \right) \text{ and } \beta = \frac{1}{2} \left(v' - 1 - n + \frac{4\delta'}{v' - 1 - n} \right)$$
(45)

$$\operatorname{coth}\left(\frac{q\mu}{2}\right) = 1 - 2z \to z = \frac{\left(1 - \operatorname{coth}\left(\frac{q\mu}{2}\right)\right)}{2} \tag{46}$$

Equation (45)-(46) in Equation (44), we obtain

$$M = \begin{bmatrix} \left(\frac{\left(1 - \coth\left(\frac{q\mu}{2}\right)\right)}{2} \right)^{\frac{1}{2}\left(\nu' - 1 - n - \frac{4\delta'}{\nu' - 1 - n}\right)} \\ \frac{1}{2} \left(\frac{\left(1 + \coth\left(\frac{q\mu}{2}\right)\right)}{2} \right)^{\frac{1}{2}\left(\nu' - 1 - n + \frac{4\delta'}{\nu' - 1 - n}\right)} \\ \frac{1}{2} F_{1}\left(a', b', c', z\right) \end{bmatrix}$$
(47)

Equation (47) was simplified to

$$M = \left(-1\right)^{\left(\frac{1}{2}(v'-1-n)+\frac{2\delta'}{v'-1-n}\right)} \frac{\left(\frac{\cos ech \frac{q\mu}{2}}{2}\right)^{v'-1-n}}{\left(\sinh \frac{q\mu}{2} - \cosh \frac{q\mu}{2}\right)^{\frac{4\delta'}{v'-1-n}}} {}_{2}F_{1}\left(a',b',c',z\right)$$
(48)

With

$$\varpi = (\nu' - 1 - n) = \left(\sqrt{\frac{2m_0V_2}{h^2} + \frac{1}{4}} - \frac{1}{2} - n\right)$$
(49)

$$\Omega = \frac{\delta'}{\left(v'-1-n\right)} = \frac{\frac{m_0}{2q^2 h^2} \left(qV_1 - q^2V_2\right)}{\left(\sqrt{\frac{2m_0V_2}{h^2} + \frac{1}{4}} - \frac{1}{2} - n\right)}$$
(50)

Equation (45) was inserted into Equation (37), we get

 $a' = \alpha + \beta - v' + 1 = -n$ (51)

$$b' = \alpha + \beta + v = 2v' - 1 - n \tag{52}$$

$$c' = 2\alpha + 1 \rightarrow c' = \left(\left(v' - 1 - n \right) - \left(\frac{4\delta'}{\left(v' - 1 - n \right)} \right) \right) + 1$$
(53)

Equation (52)-(53) was simplified using Equation (42)-(43), we get

$$b' = 2v' - 1 - n = 2\left(\sqrt{\frac{2m_0V_2}{h^2} + \frac{1}{4}} + \frac{1}{2}\right) - 1 - n = 2\sqrt{\frac{2m_0V_2}{h^2} + \frac{1}{4}} - n$$
(54)

$$c' = \left(\left(\sqrt{\frac{2m_0 V_2}{h^2} + \frac{1}{4}} - \frac{1}{2} - n \right) - \left(\frac{\frac{2m_0}{q^2 h^2} \left(q V_1 - q^2 V_2 \right)}{\left(\sqrt{\frac{2m_0 V_2}{h^2} + \frac{1}{4}} - \frac{1}{2} - n \right)} \right) \right) + 1$$
(55)

With,

$$\rho = \sqrt{\frac{2m_0 V_2}{h^2} + \frac{1}{4}}$$
(56)

Equation (49)-(50) and equation (56) were inserted into Equation (54)-(55), so we get a simpler form as follows

$$a' = -n \tag{57}$$

$$b' = 2\rho - n \tag{58}$$

$$c' = \varpi - 4\Omega + 1 \tag{59}$$

By applying Equation (14), Equation (49)-(50) and Equation (57)-(59) in Equation (48), we get

$$M = \left(-1\right)^{\left(\frac{1}{2}(\sigma)+2\Omega\right)} \frac{\left(\frac{\cos ech \frac{q\mu}{2}}{2}\right)^{\sigma}}{\left(\sinh \frac{q\mu}{2} - \cosh \frac{q\mu}{2}\right)^{4\Omega} {}_{2}F_{1}\left(a^{'}, b^{'}, c^{'}, z\right)}$$
(60)

with

$${}_{2}F_{1}(a,b,c,z) = 1 + \frac{ab}{c}z + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{z^{2}}{2!} + \dots$$
(61)

The result of the un-normalized wave function equation for the Schrodinger equation in Bispherical coordinate with the Hypergeometry method for Kratzer potential with quantum number variation (n) is shown in Table 1.

Table 1. The un-normalized wave function equation for the Schrodinger equation in Bispherical coordinate with Hypergeometry method for Kratzer potential with quantum number variation (n)





Table 1 is wave function (M_0) for ground state (n_0) , wave function (M_1) for energy level 1 (n_1) , wave function (M_2) for energy level 2 (n_2) .

4. Conclusion

The Schrodinger equation in Bispherical coordinate with Kratzer potential can be solved by using Hypergeometry. Hypergeometry method used to obtain the energy spectrum and un-normalized wave function for Schrodinger equation in Bispherical coordinate with Kratzer potential. The result of energy spectrum equation for Schrodinger equation in Bispherical coordinate with Kratzer potential can be shown in equation (41). The result of un-normalized wave function equation for Schrodinger equation in Bispherical coordinate with Kratzer potential can be shown in equation in Bispherical coordinate with Kratzer potential can be shown in Table 1.

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